KFM 14: Ferroics – Domains and Domain Walls 1

Chair: Dr. Donald Evans (Augsburg University)

Time: Wednesday 9:30–12:05 Location: H5

KFM 14.1 Wed 9:30 H5

Strain driven conducting domain walls in a Mott insulator — •Lukas Puntigam[1], Donald Evans[1], Markus Altthaler[1], Somnath Ghara[1], Lilian Prodan[1], Vladimir Tsurkan[1,2], Stephan Krohns[1], and Istvan Kezsmarki[1] — [1]Universität Augsburg, 86159, Augsburg, Deutschland — [2]Institute of Applied Physics, MD 2028 Chisinau, Moldova

Ferroelectric domain walls, which can be written, tuned or erased, are being considered as functional building blocks for nanoelectronics. Especially, conducting domain walls are of high interest to achieve this functionality. To date, the origin for increased conductivity in ferroelectrics domain walls has been typically attributed to the formation of screening charges driven by polar discontinuities.

Here, we establish that for the template system, the lacunar spinel GaV_4S_8 also strain can enhance the conductivity of specific domain walls. This system exhibits ferroelectric domain pattern below a Jahn-Teller transition at 42K. At this temperature a change in its crystal structure can result in mechanical stress at domain walls. Piezoresponse force microscopy revealed an interesting ferroelectric pattern. Each ferroelectric domain can be identified by structural considerations to be one of the four possible polar direction. In case of domain walls between structural incompatible domains measurements with conductive atomic force microscopy show strongly enhanced conductivity denoting an additional twist highly conductive domain walls. Further, spatially resolved IV spectroscopy enable the investigation of the underlying conductivity mechanism at the tip-sample interface.

KFM 14.2 Wed 9:50 H5

In-situ tracking of the evolution of polarization during the growth of layered-ferroelectric Aurivillius phases — •Ipek Efe, Elzbieta Gradauskaite, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zürich, Switzerland

The highly anisotropic nature of layered oxides is key to exotic functionalities such as superconductivity, magnetoresistance, and ferroelectricity, which are promising for applications. However, their integration in epitaxial design is challenging due to the complexity of the unit cell, which makes precise monitoring of the growth a necessity. Here, we directly access the polarization dynamics of the model system Aurivillius $Bi_5FeTi_3O_{15}$ films during the epitaxial growth using in-situ optical second harmonic generation (ISHG). We identify an oscillating intensity of the ISHG signal during two-dimensional layer-by-layer growth. We correlate these oscillations with the periodical evolution of the polarization of ferroelectric film dictated by the chemistry of the planes in the unit-cell, which consists of alternating positively charged fluorite-like $(Bi_2O_2)^{2+}$ layer and negatively charged $(Bi_3FeTi_3O_{13})^{2-}$ perovskite blocks. In combination with reflection high-energy electron diffraction, we show how polarization of the films consistently switches from an out-of-plane orientation during the perovskite blocks growth, to a fully-in-plane orientation with the completion of the unit-cell termination and the $(Bi_2O_2)^{2+}$ capping. Our findings reveal previously hidden polarization dynamics during the epitaxial design and bring new insights in the sub-unit cell control of layered oxide films properties for the development of energy efficient oxide electronics.

KFM 14.3 Wed 10:10 H5

Continuous polarization control at nanoscopic dimensions — •Martin F. Sarott[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, Empa Swiss Federal Laboratories for Materials Science and Technology, Switzerland

The switchable bistable polarization in ferroelectrics allows for the binary control of optical, electronic, and catalytic properties. Going beyond the limitation of a binary remanent polarization holds great promise for emerging neuromorphic concepts. Here, we demonstrate that we can arbitrarily set the magnitude of the remanent ferroelectric polarization at the nanoscale in epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ thin films with a single DC bias. By approaching the PZT morphotropic phase boundary, we achieve a high degree of control over this unusually susceptible system via epitaxial strain. We employ this to accomplish the formation of decoupled nanometric 180° domains with a broad coercive field distribution. Using in-situ optical second harmonic generation and X-ray diffraction, we study the emergence of the nanoscopic domain configuration. We then use piezoresponse force microscopy to demonstrate the ability to locally and reversibly modulate the remanent polarization *continuously* between depolarized and saturated, while preserving the nanoscopic length scale of the domains. We highlight the technological relevance of nanoscale non-binary polarization switching, by showing (i) the voltage-controlled tunability of the nonlinear optical response and (ii) the quasi-continuous tunability of the tunnel electroresistance in ferroelectric tunnel junctions.

KFM 14.4 Wed 10:30 H5

Impact of strontium on domain wall mobility in barium titanate — •Aris Dimou[1], Pierre Hirel[2], and Anna Grünebohm[1] — [1]Ruhr-Uni. Bochum, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Bochum, Germany — [2]Univ. Lille, Unité Matériaux et Transformations (UMET), Lille, France

Solid solutions of barium-strontium titanate are widely used, environmentally friendly ferroelectric materials that are important for a plethora of applications [1,2]. The presence of domain walls are known to change the properties of a material, and its mobility is of key interest in contemporary electronic devices [3]. Surprisingly little attention has so far been paid to the impact of Sr on the domain wall mobility in barium titanate.

Here we present a microscopic study on the case of Sr inclusions in barium titanate. Our simulations reveal an increase in the activation energy for domain wall movement at the Sr inclusion. Suggesting that a thin Sr plane is enough to pin the domain wall.

[1] Acosta et al., $BaTiO_3$-based piezoelectrics: Fundamentals, current status, and perspectives. *Applied Physics Review*, **4**, 2017.

[2] Grünebohm et al., Interplay of domain structure and phase transitions: theory, experiment and functionality. *J. Phys. L Condens. Matter*, **34**, 2022.

[3] Sharma et al., Functional ferroic domain walls for nanoelectronics. Currently. Open. *Solid State Mater. Sci.*, **9**, 2005.

15 min. break

KFM 14.5 Wed 11:05 H5

Stability of enhanced domain wall conductivity in single-crystalline lithium niobate — •Ahmed Samir Lotfy[1,2], Manuel Zahn[1], Michael Rüsing[1], and Lukas Eng[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany — [2]Department of materials, ETH Zürich, Zürich, Switzerland

Domain-wall conductivity (DWC) in ferroelectrics has emerged as a key functionality for developing nanoelectronic devices. In this regard, lithium niobate (LNO) is a promising candidate as previous studies have shown the capability to significantly enhance its DWC by making use of head-to-head and tail-to-tail DW configurations, and DW inclination angles under voltage treatments. However, understanding of the temporal and temperature-dependent stability of the enhanced DWC is lacking, limiting further steps of device implementation. For this, we performed a series of conductive atomic force microscopy and macroscopic electrometer measurements on single crystalline LNO samples. We show a characteristic conductance trend during voltage-induced enhancement which provides insights into the temporal stability of DWC. Moreover, our temperature-dependent measurements between 100 K and 300 K reveal the transport mechanism along the walls, pointing to the role of bound polarons. This is confirmed by the calculation of the activation energy. These results provide key insights into the stability of DWC in LNO for applications in practical devices.

KFM 14.6 Wed 11:25 H5

Electron scattering signatures of ferroelectric domains — •Ursula Ludacka[1], Jiali He[1], Emil Frang Christiansen[1], Shuyu Qin[2], Zewu Yan3[3,4], Edith Bourret[4], Antonius van Helvoort[1], Joshua Agar[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Department of Materials Science and Engineering, Lehigh University, Bethlehem, PA 18015, USA — [3]ETH Zurich, Zurich, Switzerland —

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The emergence of ferroelectricity originates from polar displacements of lattice atoms, connotating a one-to-one correlation between electronic and structural properties at the atomic level. An established approach that allows for determining associated structural variations is scanning electron diffraction (SED). In SED, a focused electron beam is scanned over the specimen, probing diffracted electrons at each position of the raster scan. The corresponding patterns represent unique fingerprints of the probed areas, containing structural information. We demonstrate the potential and opportunities of this innovative 4D-STEM approach using improper ferroelectric $ErMnO_3$, an ideal model system as its basic ferroelectric properties and atomic-scale structure are well understood. In the ferroelectric state, the Er ions exhibit characteristic up-up-down and down-down-up patterns, corresponding to ferroelectric 180° domains with positive and negative polarization, respectively. These shifts cause different Bragg scattering conditions for the electrons and, hence, specific diffraction patterns that we utilize for domain imaging assisted by machine learning algorithms.

KFM 14.7 Wed 11:45 H5

Oxygen vacancies nucleate domain walls in ferroelectrics — •Urko Petralanda[1], Mads Kruse[1], Hugh Simons[2], and Thomas Olsen[1] — [1]CAMD, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Domain walls are topological defects which emerge spontaneously in ferroelectrics [1]. At charged domain walls (CDW), free charge from the bulk is promoted to the conduction band through a band-bending mechanism, to compensate their local bound charge [2]. This creates highly conductive embedded mobile 2D nanosheets, suitable for nanoelectronics related applications [2]. Oxygen vacancies are believed to play a role in helping CDW overcome their strong electrostatic interaction. In this work [3], by means of density functional theory calculations in $BaTiO_3$ we clarify the screening mechanism of CDW charge in both pristine and oxygen vacancy aided cases, and we propose that, beyond the commonly accepted view of oxygen vacancies as CDW stabilizers, they can actually ignite the formation of CDW. We explain the experimentally observed difference in electronic conductivity of the positively and negatively charged CDW in $BaTiO_3$, as well as the generic prevalence of CDW in ferroelectrics. Such a vacancy driven CDW formation implies that specific charged domain wall configurations may be realized by bottom-up design.

[1] G. Catalan et al, Rev. Mod. Phys. 84, 119 (2012)
[2] T. Sluka et al, Nat. Commun. 4, 1808 (2013).
[3] U Petralanda et al, Phys. Rev. Lett. 127, 117601 (2021)